

Interference in Bohmian Mechanics with Complex Action

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Abstract

In recent years, intensive effort has gone into developing numerical tools for exact quantum mechanical calculations that are based on Bohmian mechanics. As part of this effort we have recently developed an alternative formulation of Bohmian mechanics in which the quantum action, S , is taken to be complex [JCP **125**, 231103 (2006)]. In the alternative formulation there is a significant reduction in the magnitude of the quantum force as compared with the conventional Bohmian formulation, at the price of propagating complex trajectories. In this paper we show that Bohmian mechanics with complex action is able to overcome the main computational limitation of conventional Bohmian methods — the propagation of wavefunctions once nodes set in. In the vicinity of nodes, the quantum force in conventional Bohmian formulations exhibits rapid oscillations that pose severe difficulties for existing numerical schemes. We show that within complex Bohmian mechanics, multiple complex initial conditions can lead to the same real final position, allowing for the description of nodes as a sum of the contribution from two or more crossing trajectories. The idea is illustrated on the reflection amplitude from a one-dimensional Eckart barrier. We believe that trajectory crossing, although in contradiction to the conventional Bohmian trajectory interpretation, provides an important new tool for dealing with the nodal problem in Bohmian methods.

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The challenge of performing quantum mechanical calculations on systems of many degrees of freedom has been a major focus of the theoretical chemistry community for almost four decades. Since classical mechanics can be applied to systems with tens of thousands of degrees of freedoms it is only natural that much attention has focused on methods capable of describing quantum effects but requiring only the propagation of classical trajectories. One approach that has shown significant progress in recent years is the use of Bohmian mechanics (BM)[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]. Originally developed in the 1950’s as a causal formulation of quantum mechanics (QM), in this formulation trajectories evolve in the presence of the usual Newtonian force plus an additional quantum force[13]. Although the quantum force is nonlocal, the formulation of BM in terms of trajectories suggests the possibility of achieving an efficiency that is compatible with classical trajectory methods. Despite its successes, BM suffers from several drawbacks that have prevented it from becoming an effective numerical tool to date, the most significant of these being the nodal problem — a numerical instability in regions where the wavefunction oscillates that eventually leads to a breakdown of the numerical scheme[12].

In this paper we address the nodal problem using a recently developed variation on BM that we call Bohmian mechanics with complex action (BOMCA) [14, 15], where the phase S , is taken to be complex. Like conventional BM, BOMCA is formally identical to the exact Schrödinger equation; however the quantum force is significantly smaller and more localized than in conventional Bohmian mechanics. This comes at the expense of the trajectories being complex.

In our previous publication[14] we focused on the transmitted part of a wavepacket scattered from an Eckart barrier; we demonstrated tunneling probabilities that were in virtually perfect agreement with the exact quantum mechanics down to 10^{-7} . Here we complete the picture by calculating the reflected part of the wavefunction. Whereas the transmitted part is nodeless, the reflected part, for a wide range of energies, has an oscillatory structure. We show that the oscillatory structure is obtained automatically in BOMCA simply by including the contributions from multiple initial conditions that lead to the same final position.

The origin of the nodal problem in BM can be traced back to the hydrodynamic equations of QM, which constitute the first step in the derivation of the Bohmian formulation. In

conventional BM these equations take the form:

$$S_t + \frac{S_x^2}{2m} + V = -Q, \quad (1)$$

$$A_t + \frac{1}{m}A_x S_x + \frac{1}{2m}A S_{xx} = 0, \quad (2)$$

where $V(x, t)$ is the potential of the system, m is the mass of the particle, \hbar is Planck's constant divided by 2π and the subscripts denote partial derivatives.

$$Q \equiv -\frac{\hbar^2}{2m} \frac{A_{xx}}{A} \quad (3)$$

is referred as the “quantum potential”. As can be seen from the expression for Q , the quantum potential diverges at nodal regions of the wavefunction. Numerically the difficulty is even more severe — well before a node is formed, when the amplitude of the wavefunction exhibits only nodeless ripples, the quantum trajectories are highly unstable due to rapid oscillations in the quantum potential[12].

Since nodes in quantum mechanics arise from interfering amplitudes, it is only natural to attempt to solve the nodal problem by applying the superposition principle — to decompose the wavefunction into two nodeless parts and to propagate each part separately using trajectories. Indeed, two such methods have been developed, the Counter Propagating Wave Method (CPWM)[9] and the Covering Function Method (CFM)[10]. However, since nodeless wavefunctions do not stay nodeless for a general potential, these methods generally require a series of time-dependent decompositions of the total wavefunction, which is numerically inconvenient and largely arbitrary.

A somewhat more natural strategy to solve the nodal problem is to apply the superposition principle directly to the contribution of the quantum trajectories. The superposition of contributions from multiple trajectories is a central concept in the semiclassical literature[16]; however, in conventional BM, the crossing of trajectories in configuration space is strictly prohibited. Indeed, the “no-crossing” rule plays a central role in conventional BM: if trajectories could cross it would undermine the Bohmian interpretation of QM, in which the quantum trajectories are candidates for the actual trajectory on which a particle propagates in space. Since the BOMCA formulation yields generally an approximation to QM, trajectories are allowed to cross. In this paper we demonstrate how combining the contributions of crossing trajectories yields accurate interference patterns.

The starting point of the BOMCA formulation[14] is the insertion of the ansatz[17, 18, 19, 20] $\psi(x, t) = \exp \left[\frac{i}{\hbar} S(x, t) \right]$ in the time-dependent Schrödinger equation, where we allow the phase to be *complex*. This yields a *single* quantum complex Hamilton-Jacobi equation[17, 18, 19, 20]

$$S_t + \frac{1}{2m} S_x^2 + V = \frac{i\hbar}{2m} S_{xx}, \quad (4)$$

In the spirit of conventional BM our aim is to solve eq.(4) in the Lagrangian approach, that is along quantum trajectories. A quantum trajectory is defined by

$$\frac{dx}{dt} = v(x, t); \quad v(x, t) \equiv \frac{1}{m} S_x(x, t). \quad (5)$$

Due to the definition of x as time-dependent in eq.(5), we write the solutions of this equation as $x(t; x_0)$ where x_0 is the starting point of the trajectory. Unlike conventional BM, the complex value of S yields quantum trajectories $x(t; x_0)$ that evolve in the complex plane. A Newtonian-like equation of motion for $v(x, t)$ is obtained by taking a spatial derivative of eq.(4) and applying eq.(5); after a short manipulation we obtain

$$\frac{dv[x(t; x_0), t]}{dt} = - \underbrace{\frac{V_x}{m}}_{F_c/m} + \underbrace{\frac{i\hbar}{2m} v_{xx}}_{F_q/m}, \quad (6)$$

where we identify F_c , F_q as the classical and the quantum force respectively. The presence of v_{xx} in the quantum force term prevents the first equation in (5) and eq.(6) from being a closed set.

We tackle the problem of calculating v_{xx} along a trajectory by taking iterated spatial partial derivatives of eq.(6). After a short manipulation the result can be written as

$$\frac{dv^{(n)}}{dt} = - \frac{V^{(n+1)}}{m} + \frac{i\hbar}{2m} v^{(n+2)} - \tilde{g}_n; \quad n = 0, \dots, \infty, \quad (7)$$

where $\tilde{g}_0 = 0$ and $\tilde{g}_n = \sum_{j=1}^n \binom{n}{j} v^{(j)} v^{(n-j+1)}$ for $n \geq 1$. Here $v^{(n)}$ denotes the n^{th} spatial derivative of v . A similar procedure was used in Refs.[2, 3, 4] in conventional BM. The set of eqs.(7) and the first equation in (5) are now an infinite but closed set that describes a *fully local* complex quantum trajectory. We may obtain a numerical approximation by truncating the infinite set at some $n = N$, thus replacing eq.(6) with a system of $N + 1$ coupled ODEs. Since each equation of motion for $v^{(n)}$ in (7) depends on the subsequent $v^{(n+2)}$, the truncation is done by setting $v^{(N+1)} = v^{(N+2)} = 0$. The initial conditions for the

$v^{(n)}$'s are given by

$$v^{(n)}(0; x_0) = \frac{1}{m} \frac{\partial^n S_x(x, 0)}{\partial x^n} \Big|_{x=x_0} = \frac{\partial^n}{\partial x^n} \left[-i\hbar \frac{\psi_x(x, 0)}{\psi(x, 0)} \right] \Big|_{x=x_0}, \quad (8)$$

where we have applied the definition from (5) together with $S = -i\hbar \ln \psi$, the latter following from the original ansatz. x_0 is the initial position of an arbitrary single trajectory, which is generally complex. The equation of motion for the action along a trajectory is similar to its classical counterpart, with the addition of the quantum potential:

$$\frac{dS[x(t; x_0), t]}{dt} = S_t + vS_x = \frac{1}{2}mv^2 - V + \frac{i\hbar}{2}v_x. \quad (9)$$

Solving for S and inserting the result into the original ansatz yields the wavefunction $\psi[x(t; x_0), t] = \exp \{ \frac{i}{\hbar} S[x(t; x_0), t] \}$ at position $x(t; x_0)$ in the complex plane. In Ref. [14], we discussed the practical issue of finding trajectories that end up on the real axis $x(t_f; x_0) \in \mathbb{R}$ at t_f . Once these trajectories are found, the wavefunction on the real axis $\psi[x(t_f; x_0), t_f]$ is reconstructed.

As a numerical example, consider the one-dimensional scattering of an initial Gaussian wavepacket $\psi(x, 0) = (2\alpha/\pi)^{1/4} e^{[-\alpha(x-x_c)^2 + \frac{i}{\hbar} p_c(x-x_c)]}$ from an Eckart potential $V(x) = D/\cosh^2(\beta x)$. We take $x_c = -0.7$, $\alpha = 30\pi$, $D = 40$, $\beta = 4.32$ and $m = 30$ (all units are atomic units). The system is the same as in our previous publication[14]. The average translational energy of the initial Gaussian is taken as $E = p_c^2/m = 10 < D$. We focus on trajectories that end up at a final time $t_f = 0.995$ with $x(t_f) < 0$, and thus contribute to the reflected part of the wavefunction. t_f is chosen as sufficiently long for the wavepacket to scatter from the barrier and interference effects to appear. First we focus on the $N = 1$ BOMCA approximation, for which the equations of motion are:

$$\frac{dx}{dt} = v, \quad \frac{dv}{dt} = -\frac{V_x}{m}, \quad \frac{dv_x}{dt} = -\frac{V_{xx}}{m} - v_x^2, \quad (10)$$

with the auxiliary eq.(9). Note that the $N = 1$ trajectories obey Newton's equations of motion. As indicated in Ref. [14], eqs.(10) are closely related to Generalized Gaussian Wavepacket Dynamics (GGWPD)[21], which also uses complex trajectories. As a result, many of the insights in Ref. [21] concerning multiple root trajectories can be carried over to the case of complex Bohmian mechanics, although we have found that the structure and the number of the root branches generally depend on the value of N , the order of truncation.

In fig.1 we plot three branches that contribute to the reflected wavefunction. A branch is defined as the locus of *initial* positions of trajectories that end at time t_f at real x_f with

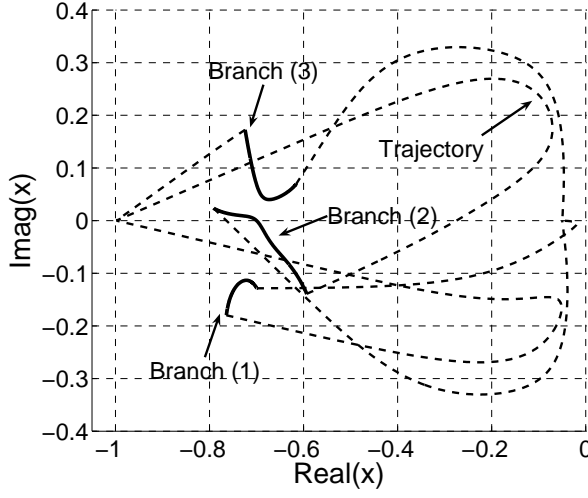


FIG. 1: Scattering of a Gaussian from an Eckart potential barrier within the $N=1$ BOMCA approximation (the parameters are given in the text). Three branches and six sample complex trajectories are depicted. The branches are the locus of initial positions of trajectories that end at time $t_f = 0.995$ at real x_f , $-1 < x_f < -0.05$, and thus contribute to the reflected wavefunction. The figure shows two sample trajectories emerging from each branch, one that ends at $x_f = -1$ and one that ends at $x_f = -0.05$.

x_f corresponding to a reflected segment of the wavefunction, $x_f \in [-1, -0.05]$. Two sample trajectories are depicted emerging from each branch, one that ends at position $x_f = -1$ and one that ends at $x_f = -0.05$. Thus, to each final position (for this segment of the reflected wavefunction) there correspond three initial positions — one originating from each of the three branches — and the wavefunction should therefore include contributions from all three branches. As in Ref. [21], at short times only one branch contributes to the final wavefunction. We refer to this branch as the “real branch” since it incorporates a trajectory that stays on the real axis at all times (the trajectory that initiates from $x_0 = x_c$). At longer times, secondary branches begin to make a significant contribution to the final wavefunction. There is apparently no fundamental limitation on the number of the secondary branches, although in the section of the complex plane depicted in fig.1 no other branches were found. In fig.1, branch (2) is the real branch while branches (1) and (3) are secondary branches.

In fig.2(a) we plot $|\psi_j(x, t_f)| = |\exp[iS_j(x, t_f)/\hbar]|$, $j = 1, 2, 3$, where j corresponds to each of the three branches. In fig.2(b) we present the result of adding pairs of branches,

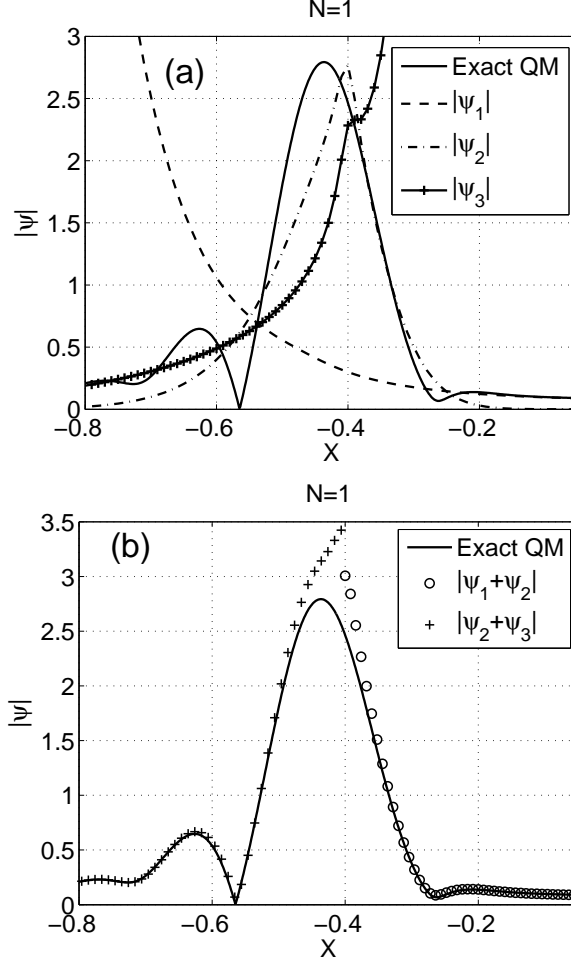


FIG. 2: (a) $N = 1$ BOMCA approximation corresponding to each of the three branches $j = 1, 2, 3$ (see fig.1), $|\psi_j(x, t_f)| = |\exp[iS_j(x, t_f)/\hbar]|$. In the region of the transmitted wavefunction (starting from $x \approx -0.2$), a good approximation to the exact result is obtained by just a single branch (branch (1)). (b) The result of adding contributions from pairs of branches $|\psi| = |\psi_j + \psi_i|$, $i \neq j$. Different choices of i and j are useful in different regions of the wavefunction.

$|\psi| = |\psi_j + \psi_i|$, $i \neq j$. We see that to a good approximation the rippled parts of the wavefunction are described by a simple superposition with a proper choice of i and j .

Note that as we approach the region of the transmitted part of the wavefunction ($x \gtrsim -0.2$) a *single* branch (branch (1)) is enough to provide a good approximation. In fact, this is the branch that is responsible for the transmitted wavefunction ($x_f > 0$, not shown), and hence we will call this the "transmitted branch". At energies on the order of magnitude of the barrier height, the "transmitted branch" is the real branch, but at lower energies (and

longer time scales) there is a crossover and the transmitted branch is one of the secondary branches. The existence of a single transmitted branch coincides well with the nodeless character of the transmitted part of the wavefunction. By the same token, in Ref. [14] we showed that the reflected part of the wavefunction can be well approximated by a single branch if it has no ripples or nodes.

The issue of which branches should be included in the sum and when, is obviously of central importance to the method; at present, we do not have a rigorous justification for the neglect of certain branches. A partial discussion is given in Ref. [21] in the context of GGWPD, but the BOMCA formulation, being more general, requires a more comprehensive discussion, which we leave to a future publication.

We now turn to the next order of approximation, $N = 2$. The equations of motion are based on eqs.(10) with two changes. The second equation in (10) is replaced with eq.(6), in which there is a quantum force. Knowledge of the quantum force requires an equation of motion for v_{xx} . We derive such an equation by inserting $n = 2$ in eqs.(7) and taking $v^{(4)} = 0$, leading to

$$\frac{dv_{xx}}{dt} = -\frac{V_{xxx}}{m} - 3v_x v_{xx}. \quad (11)$$

At the level of $N = 2$, four branches contribute to the reflected wavefunction at t_f . Fig.3(a) depicts the contribution of the four branches, $|\psi_j|$, $j = 1, \dots, 4$. The result of adding pairs of branches $|\psi| = |\psi_j + \psi_i|$, $i \neq j$ is given in fig.3(b). There is a significant increase in accuracy relative to $N = 1$ in the vicinity of the maximum and to its right, although there is a slight decrease in accuracy relative to $N = 1$ to the left of the maximum.

In conclusion, we have demonstrated that BOMCA accounts for interference and nodal structures of wavefunctions in a simple and natural way. In spite of the conceptual difficulties that crossing trajectories may pose for BM as an interpretational tool of QM, this notion introduces a powerful numerical tool and might even enrich the orthodox interpretation of the Bohmian formulation. The present results, combined with the simple and accurate results obtained for tunneling in Ref. [14], demonstrates great promise for BOMCA as a versatile alternative to current semiclassical methods. As mentioned above, several issues require a more comprehensive understanding. First, what are the convergence properties of the method as higher order approximations are taken to the quantum force, that is increasing the value of N ? Can rigorous rules be derived for the summation of the different branches? What is the relation between the exact phase that diverges at a node and the approximate

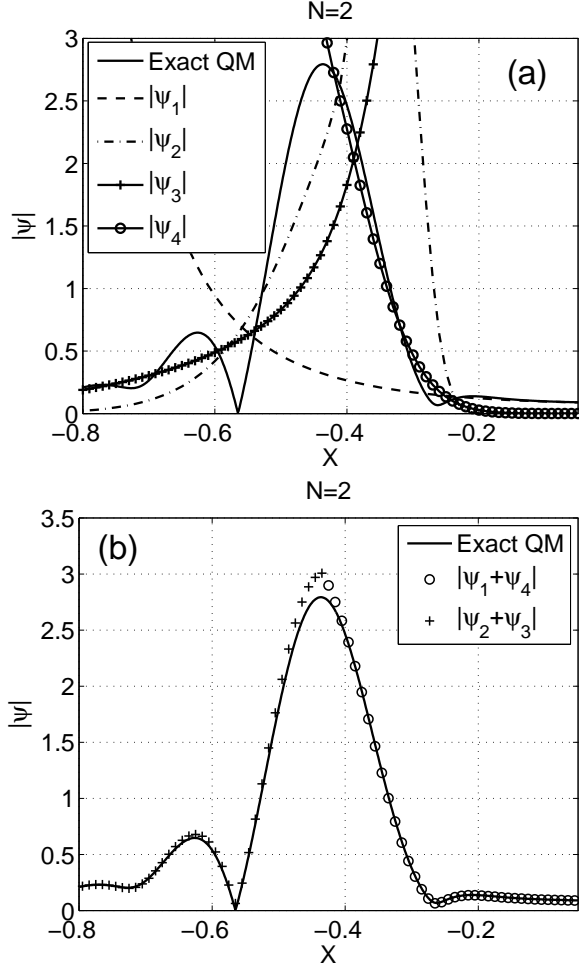


FIG. 3: (a) $N = 2$ BOMCA approximation corresponding to four branches $|\psi_j(x, t_f)| = |\exp[iS_j(x, t_f)/\hbar]|$, $j = 1, \dots, 4$. (b) The result of adding contributions from pairs of branches $|\psi| = |\psi_j + \psi_i|$, $i \neq j$. Except for a slight decrease in accuracy left to the maximum, the results for $N = 2$ where a quantum force term is added are better than for $N = 1$ (complex classical trajectories).

BOMCA formulations that can account for nodes via a bipolar or multipolar expansion? We intend to address all these questions in future work. This work was supported by the Israel Science Foundation (576/04).

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